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Recognition for scientific, technical achievements

Carlos Tomé selected for plasticity research medal

The International Journal of Plasticity will honor Carlos Tomé (Materials Science in Radiation and Dynamics Extremes, MST-8) with the Khan International Medal during the 2016 International Conference on Plasticity, Damage and Fracture, being held in January in Hawaii. The journal recognized him for his "outstanding life-long contributions in the field of plasticity."

Upon hearing of his award, Tomé acknowledged his work with DOE Basic Energy Sciences, the Consortium for Advanced Simulation of Light Water Reactors, and the Advanced Simulation and Computing Program that provided the "continuity, exposure, and interactions with first-class research-



ers," which he said made possible his contributions to the field of plasticity.

Tomé will deliver a plenary lecture, "Recent Advances in Modeling the Constitutive Response of Aggregates," at the upcoming conference and will write a review paper for the journal. A mini-symposium, "Stochastic Information in Characterization and Modeling of Mechanical Behavior," will

be organized in his behalf for the 2017 International Plasticity Conference, and a special issue of the journal will include the symposium presentations.

Tomé earned a PhD in physics from the National University of La Plata, Argentina, and joined the Laboratory in 1996. He pioneered the theoretical and numerical development of physically based modeling of mechanical behavior of polycrystals, with a focus on the role played by texture, twinning, and microstructure on the anisotropic properties of engineering and geologic materials. Such approaches have led to revolutionary changes in how simulations and interpretation of measurements on mechanical behavior are

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Lily Wang awarded for contributions to material aging assessment

Metallurgy (MST-6) scientist Lily Wang was recently recognized for her efforts over the past three years on a program to understand baseline properties and aging effects on Seabreeze and diallyl phthalate for use in the B61 Life Extension Program.

Wang and her team members Diana Honnell, John Bernal, and Bo Folks in MST-6 completed the wide-ranging task of receiving classified components from the Y-12 National Security Complex in Tennessee, preparing samples for material property measurements, and executing complex accelerated aging program and characterization work on samples.

According to Art Nobile, an R&D engineer in B61-12 Life Extension Program (W-15), the program, which involved approximately 200 samples with characterization work performed in five Laboratory groups, went flawlessly. With the materials' properties well characterized, researchers are learning much about the effects of aging on them.



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From David's desk ...

Diversity and MST Division

“
I have challenged my management team to encourage diverse applicants to apply for positions and to begin having similar conversations with our pipeline network—encouraging our collaborators to help train a diverse pool from which we can recruit.”

The diversity of our workforce is a critical component of an environment leading to creative and innovative ideas. The ability to form large, multidisciplinary teams to tackle complex problems is one of the strengths at Los Alamos and MST Division. To ensure these teams develop the most innovative ideas, we need to bring together people with diverse backgrounds to help the team view the problem from multiple perspectives.

Many factors contribute to the diversity of the team including gender, ethnicity, and education/training background. As part of MST's commitment to improving the diversity of our workforce, we are following the example set by ADEPS and much of industry by posting our ethnicity and gender diversity statistics on our internal website at int.lanl.gov/org/padste/adepts/mst/diversity.shtml. Clearly, we still have work to do to improve across all job categories.

Changing the diversity of our workforce cannot be accomplished overnight, but requires a sustained commitment. Our strategy is two-fold: 1) focus on improving the diversity of our hiring pipeline and 2) raise awareness to potential unconscious bias during promotions and hiring of higher-level positions. I have challenged my management team to encourage diverse applicants to apply for positions and to begin having similar conversations with our pipeline network—encouraging our collaborators to help train a diverse pool from which we can recruit.

Lastly, we also need to ensure that our work environment supports and encourages this diverse workforce. Along these lines, we are looking for ideas that you may have for improving our work environment. If you have ideas, please raise them with your team leader, group leader, or bring them to the Division Office.

Thanks,

MST Division Leader David Teter

Tomé cont.

conducted. Material scientists and engineers in academia, national laboratories, and industry use his theories, models, and numerical codes. Tomé has published more than 170 papers in international journals, with more than 11,500 citations, and he co-authored the books *Texture and Anisotropy* and *Fundamentals and Engineering of Severe Plastic Deformation*. He received the 2013 Distinguished Scientist/Engineer Award presented by the Structural Materials Division of The Minerals, Metals & Materials Society (TMS). His work was the focus of a 2011 TMS symposium, the proceedings of which are compiled in a special issue of *Modeling and Simulation in Materials Science and Engineering*.

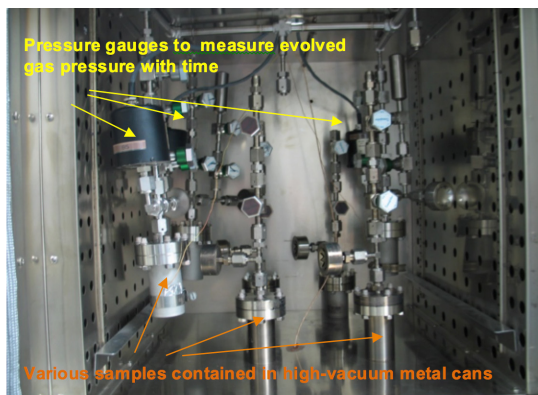
The Khan International Medal is named after *International Journal of Plasticity* Editor-In-Chief Akhtar Khan. The committee selects people they regard as having produced work that influences future research directions in the mechanics of materials.

Technical contact: Carlos Tomé

Wang cont.

Wang received a Laboratory Spot Award for her work, which included supervising, coordinating, and providing careful attention to the many elements involved in the project, while being mindful of the work's environment, safety, and health aspects to ensure workers' safety. Her contribution included managing classified component handling; coordinating sample preparation efforts; developing an experimental matrix for sample exposure; aging of samples in multiple ovens with instrumentation and data acquisition hardware; maintaining sample environments; managing laboratory facilities with gloveboxes and other complex equipment; performing characterization work on samples at the Sigma Complex; and managing the distribution of samples to four other Laboratory groups for characterization before and after aging.

The B61 gravity bomb system, deployed since 1968, is one of the oldest and most versatile weapons in the stockpile. The B61 can be carried by several different United States and NATO aircraft, and hold at risk a wide variety of targets. Los Alamos, as the design laboratory for the B61 nuclear explosive package, is working with Sandia National Laboratories to execute this life extension project.



A long-term thermal aging run: Samples were contained in sealed vacuum cans and placed in an oven for aging.

Los Alamos makes depleted uranium targets for NNSA Global Threat Reduction Initiative

Supports production of critical medical isotope in United States without weapons-grade uranium

The wonder isotope used in more than 80,000 medical imaging procedures every day to diagnose heart disease, cancer, and other conditions has a sore point: it's manufactured using highly enriched uranium, a weapons-grade material. In 2012, Congress passed the American Medical Isotopes Production Act to support domestic projects that can produce molybdenum-99 (Mo-99) with low enriched uranium instead. Mo-99 is a radioisotope that decays into technetium-99m (Tc-99), the most commonly used medical isotope.

For one such project, called mini-SHINE, the Metallurgy Group (MST-6) recently fabricated 21 clad depleted uranium (DU) targets at the Sigma Complex. Los Alamos was chosen for the work given its expertise in uranium processing and capabilities in making parts for experiments. Sigma offers casting, machining, welding, cleaning, and bonding of uranium materials, as well as characterization of uranium structure.

The targets have been approved for use in Argonne National Laboratory's mini-SHINE demonstration of producing and purifying molybdenum-99 (Mo-99) from low enriched uranium, a joint effort with SHINE Medical Technologies. The National Nuclear Security Administration's Office of Material Management and Minimization, Office of Conversion funded the work. The program helps international isotope producers convert to low enriched uranium targets, which are not useful for weapons, and encourages the establishment of Mo-99 production in the United States. Currently, Canada is the main Mo-99 producer.

The SHINE approach, which is being developed by Morgridge Institute for Research, creates Mo-99 using a sub-critical aqueous solution of low enriched uranium at the Argonne Low Energy Accelerator Facility, where the fission reaction takes place. The mini-SHINE experiments, with DU targets, seek to understand the solution chemistry and the retrieval of Mo-99.

The disks consist of a DU core clad with zircaloy: they were fabricated at Los Alamos to yield a mechanically sound and high quality bond between the uranium core and the zircaloy cladding. The final mini-SHINE assemblies are 2.1-inch-diameter disks of two thicknesses to accommodate the process assembly. The DU disks were assembled as a core DU disk inserted into two machined zircaloy can plates. The DU core and the zircaloy cans were electro-discharge machined per Argonne National Laboratory specifications, including dimensional, flatness, and out-of-round tolerances less than 0.01 inches and surface finish of 63 Ra-min. Cleaning of all components was optimized to ensure bond-

continued on page 4

Targets cont.

ing of the DU/zircaloy interface and included Blue Gold cleaner, sodium hydroxide, nitric acid, nitric acid, and ammonium bi-fluoride. Los Alamos made a single circumferential electro-beam weld on the outer edge of each disk. The can components have a step joint to facilitate assembly and to provide proper alignment for electro-beam welding. Finally, Los Alamos performed hot isostatic pressing of the DU disks to create a strong bond at the DU/zircaloy interface to aid in heat transfer.

The Los Alamos team made two DU disk assemblies for the developmental phase to analyze the DU/zircaloy bond, resulting in quality bonding and precise final dimensions of both the thin and thick disks.

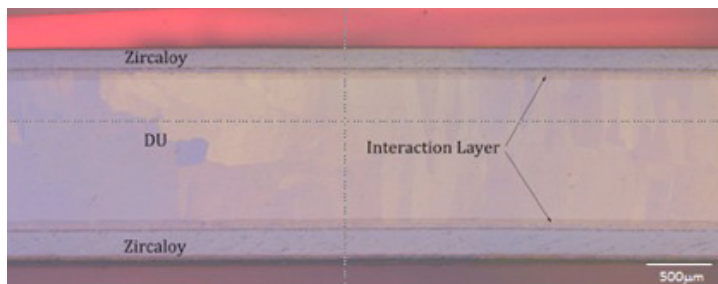
Ultrasonic testing inspection result shows bonded areas and less bonded areas on all 21 DU disks. For thin assemblies, at least 99.5% of DU/zircaloy interfaces were bonded and for thick assemblies, at least 95% of DU/zircaloy interfaces were bonded. After Argonne compared the results of each DU disk to the thermal stress analysis report that evaluates the effect of non-bonds on target life, all 21 disk assemblies were approved for use in the mini-SHINE assembly.

David Alexander, Maria Peña, Matthew Dvornak, Donald Bucholz, Dave Dombrowski, Beverly Aikin, Bo Folks, Joel Montalvo, Victor Vargas, Michael Mauro, and Pallas Papin, representing all MST-6 teams (Powder Metallurgy and Processing, Forming and Machining, Welding and Joining, Foundry, Characterization and Special Projects, Electrochemistry and Corrosion), participated in the fabrication. So did Debra Summa (Non-Destructive Testing & Evaluation team, AET-6).

This work supports the Lab's Global Security and Energy Security mission areas and the Materials for the Future science pillar. Deborah Dale (Nuclear Engineering and Nonproliferation, NEN-DO) is the Los Alamos Material Management and Minimization (NA-23) program manager.

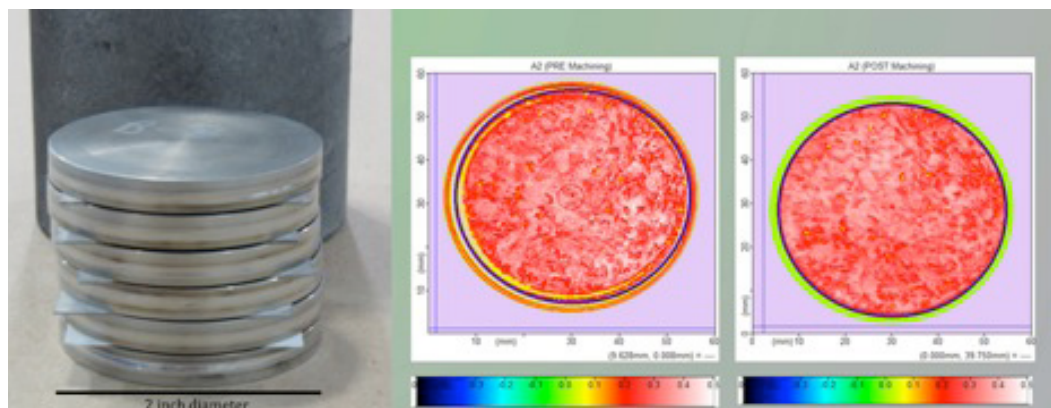
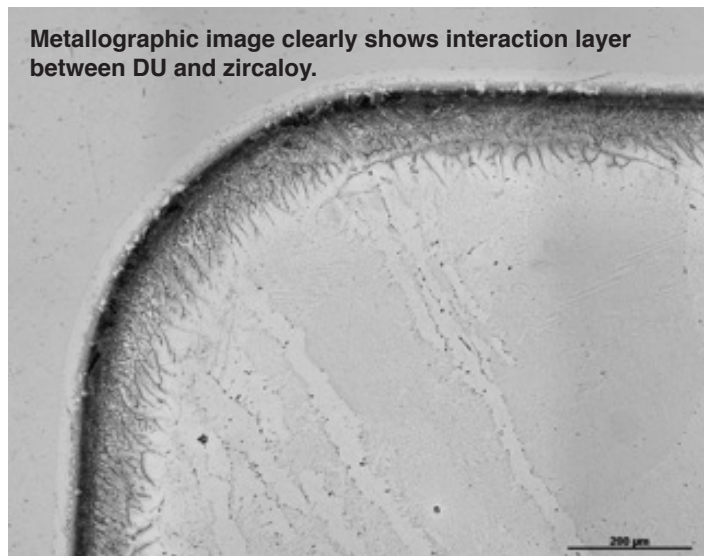
Technical contact: Maria Peña

Zircaloy DU disk edge showing electro-beam weld on zircaloy.



Microscopy image of thin development DU disk showing interaction layer between DU and zircaloy.

Metallographic image clearly shows interaction layer between DU and zircaloy.

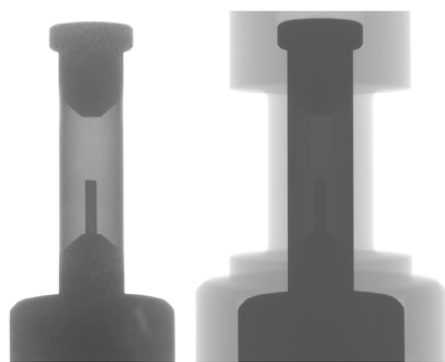


Disks after hot isostatic pressing and typical ultrasonic testing results showing bonded (red) and less bonded (yellow) areas.

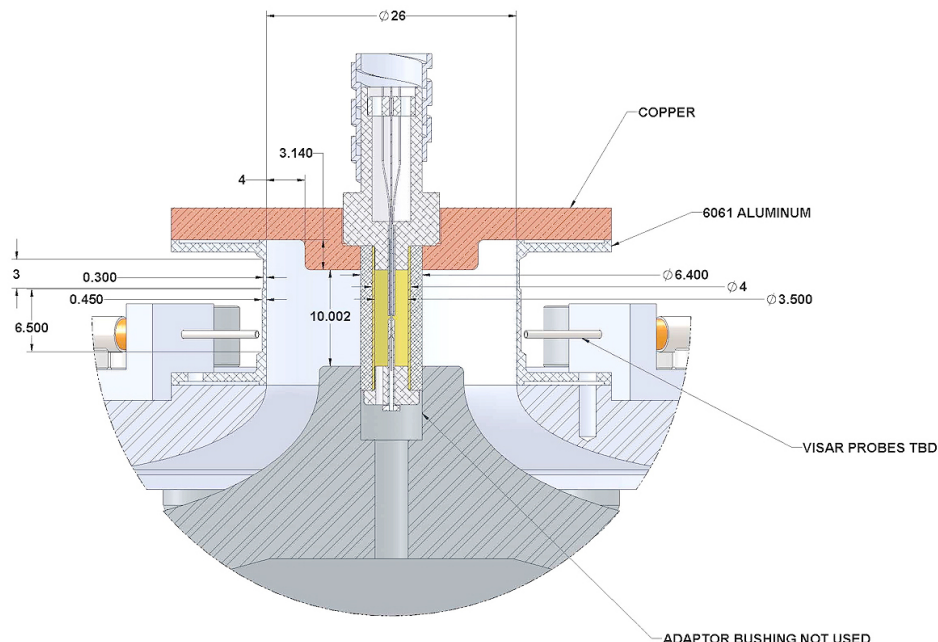
Z Machine cylindrical compression experiments on depleted uranium

Researchers executed the first containment experiment (Shot #2824) using depleted uranium in a thin walled cylindrical geometry at Sandia National Laboratories' Z machine. The team developed a new experimental geometry to acquire quasi-isentropic (nearly constant entropy) compression data at significantly higher peak pressures than previously achievable.

Los Alamos National Laboratory, General Atomics, and Sandia National Laboratories (SNL) collaboratively designed and fabricated the depleted uranium target (see figure). The extreme length-to-diameter aspect ratio required the depleted uranium blanks to be formed by electric discharge machining at Los Alamos. General Atomics precision machined the depleted uranium blanks to final specification and fabricated the target. Key to the success of these experiments was fine-grained uranium, which mattered due to the constrained geometry of these shots. The 15-mm-long cylindrical target was composed of an inner liner made of depleted uranium (inner radius 1.75 mm, 250 μ m wall thickness), and an outer liner (the pusher) made of aluminum (inner radius 2.0 mm, 1200 μ m wall thickness) that



Radiographic images of the target assembly taken at two different contrast or intensity levels. (Left): Image showing semi-transparent depleted uranium thin walled cylinder. Fiber optic probe for PDV diagnostics can be seen through target center. (Right): Image showing semi-transparent aluminum liner or "pusher" with depleted uranium thin walled cylinder appearing as fully dense solid.



Cutaway cross-section image developed during the depleted uranium target design project phase depicts the experimental configuration of the target assembly. The platform has cylindrical symmetry. The crosshatched gold region (image center) represents the depleted uranium target. The crosshatched gray region that borders it represents the aluminum liner or "pusher." (All dimensions are in mm.)

contained the electrical current and magnetic field throughout the implosion.

The diagnostics included six internal photon Doppler velocimetry (PDV) probes to measure the response of the depleted uranium inner surface to the pressure drive, six velocity interferometer system for any reflector (VISAR) probes, and two PDV probes that measure the velocity of the external surface of the aluminum anode can. All internal PDV probes returned excellent data. The depleted uranium liner was tracked to the maximum possible velocity and was quasi-isentropically compressed to the peak pressure predicted via magnetohydrodynamics simulation. Radiologic containment during dynamic actinide (i.e., uranium, plutonium, etc.) experiments on the Z machine is dependent on a set of explosively driven ultrafast closure valves. As predicted, Shot #2824 contained the uranium in the chamber.

Los Alamos and SNL have collaborated on actinide dynamic experiments

for more than 10 years. This new experimental configuration will facilitate the exploration of actinides behavior to significantly higher pressures and densities. The kind of data obtained for the validation equation of state and other physics performance properties is an example of Science on the Roadmap to MaRIE (Matter-Radiation Interactions in Extremes), the Laboratory's proposed experimental facility for control of time-dependent material performance. Similar studies could be performed at unprecedented scales using MaRIE's advanced capabilities.

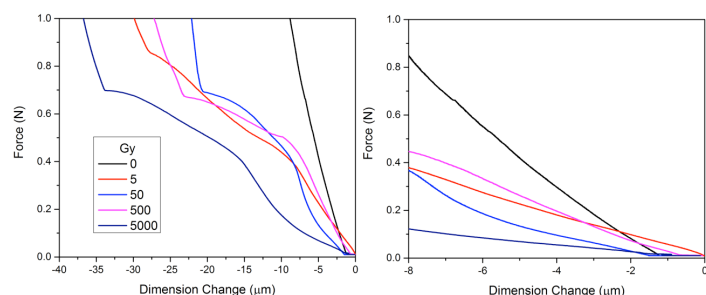
The Los Alamos team includes: Franz Freibert (Nuclear Materials Science, MST-16), Nenad Velisavljevic (Shock and Detonation Physics, M-9), and David Alexander (Metallurgy, MST-6). NNSA Defense Programs funded the research through the Dynamic Materials Properties Science Campaign. The work supports the Lab's Materials for the Future science pillar.

Technical contact: Franz Freibert

Radiation-induced spectroscopic changes in parylene-C

Parylene-C has a long history of use in medical devices, and several studies have evaluated the effects of radiation sterilization procedures on the polymer. These sterilization procedures expose a material to a single large radiation dose (\sim Mrad), and the material is evaluated for performance after the exposure. However, there has been a general lack of systematic radiation damage studies on parylene-C that cover a wide range of doses.

Engineered Materials (MST-7) researchers have undertaken a study that will evaluate, mechanically and spectroscopically, the material response of parylene-C to a wide range of radiation doses. By using a thermomechanical analyzer (TMA, TA Q400EM) under compression mode to measure the stress-strain behavior of parylene-C films, scientists can minimize the sample geometry dependence seen in previous studies that used dynamic mechanical analysis (DMA) and tensile measurements.



TMA stress-strain curves for parylene-C after various radiation doses. Left: Full scale. Right: Linear viscoelastic region.

Preliminary results from scoping studies for this project show the TMA curves, which determine the appropriate dose levels for a more detailed study. While the full stress-strain curves show dynamic differences as a function of radiation dose (see figure above), the graph on the right shows the more interesting linear viscoelastic region for the samples where the slope reveals the modulus of the material. Parylene-C becomes softer after even mild radiation doses (5 Gy), but the trend is not clear. The material is significantly harder after a 500 Gy dose, but then becomes significantly softer after a 5000 Gy dose. Such a result implies that different mechanisms (i.e., chain scission and cross linking) become dominant in different dose regimes, and future studies will pinpoint the dose ranges where competing mechanisms are dominant.

While the mechanical behavior of parylene-C as a function of radiation is the most important result, the researchers also want to understand the specific chemical and molecular changes that lead to the mechanical effects. For this purpose, they will employ a two-dimensional Fourier transform

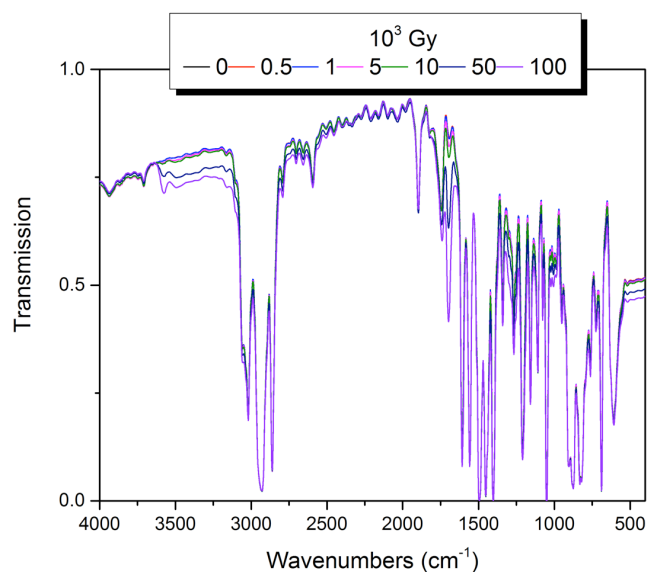
infrared (FTIR) spectroscopy technique, where a large number of spectra (200 or more) are evenly spaced over a variable range (dose range in this case) and statistical analysis allows them to identify subtle changes in the spectroscopic signature.

To establish the dose range, they measured FTIR spectra after a wide range of radiation exposures. The figure below shows that spectral changes become obvious at doses of 50 and 100 kGy, with noticeable changes near 1750 and 1300 cm^{-1} (likely carbonyl groups) and 3000-3500 cm^{-1} (typical of general oxidation). Based on these results, they will measure FTIR spectra after 500 Gy dose increments up to 100 kGy and analyze the results with specially designed algorithms.

The researchers involved are Joseph Torres, Matt Herman, Michael Blair, Rob Gilbertson, Nick Parra-Vasquez (MST-7), Nick Smith (Production Liaison, W-8), and Dave Ceman (Detonator Technology, W-6).

This work was funded by the B61-12 Life Extension Program (Program Manager Patti Buntain) and supports the Materials for the Future science pillar through an increased understanding of how radiation-induced defects are manifested and affect material performance.

Technical contact: Michael Blair

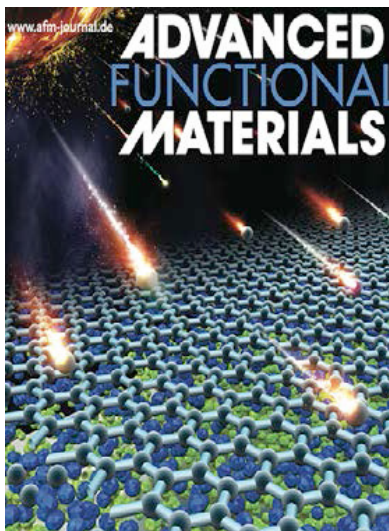


FTIR spectra of parylene-C for various doses.

Ion implantation enables synthesis of layer-tunable graphene

A new layer-tunable graphene synthesis method, developed in part at Los Alamos's Ion Beam Materials Laboratory, has the potential to be used in large-scale production lines and speed the application of graphene in nanoelectronics.

Advanced Functional Materials published the research and featured a figure from the work on the back cover.



The journal's back cover features a schematic of the ion implantation process.

Graphene, a strip of pure carbon one atom thick, is stronger than steel and is an outstanding conductor of electricity and heat.

Incorporating this material into real-world applications has proved challenging because the common production method, chemical vapor disposition, is cumbersome, expensive, and toxic. The authors report an ion implantation method that is simpler and offers precise control of graphene thickness, a crucial experimental parameter related to the physicochemical properties of graphene.

Yongqiang Wang (Materials Science in Radiation and Dynamics Extremes, MST-8) used an ion implanter at the Lab's Ion Beam Materials Laboratory to insert the required number of carbon atoms to form single-layer and double-layer graphene on a copper-nickel substrate. Selection of specific ion energy and fluence enables ion implantation to deliver the exact number of foreign atoms at a precise location within the host material matrix. Implanted carbon atoms expelled during the growth process produce high-quality graphene with the desired number of layers, typically single or double layers. Theoretical calculations confirmed the growth mechanism. This is the first investigation of the use of a dual metal substrate combined with ion implantation for the synthesis of layer-tunable graphene. Because ion implantation is a core technology in microelectronics processing, this method could be implemented into production lines and to expedite the application of graphene to nanoelectronics.

Reference: "Synthesis of Layer-Tunable Graphene: A Combined Kinetic Implantation and Thermal Ejection Approach," *Advanced Functional Materials* **25**, 3666 (2015).

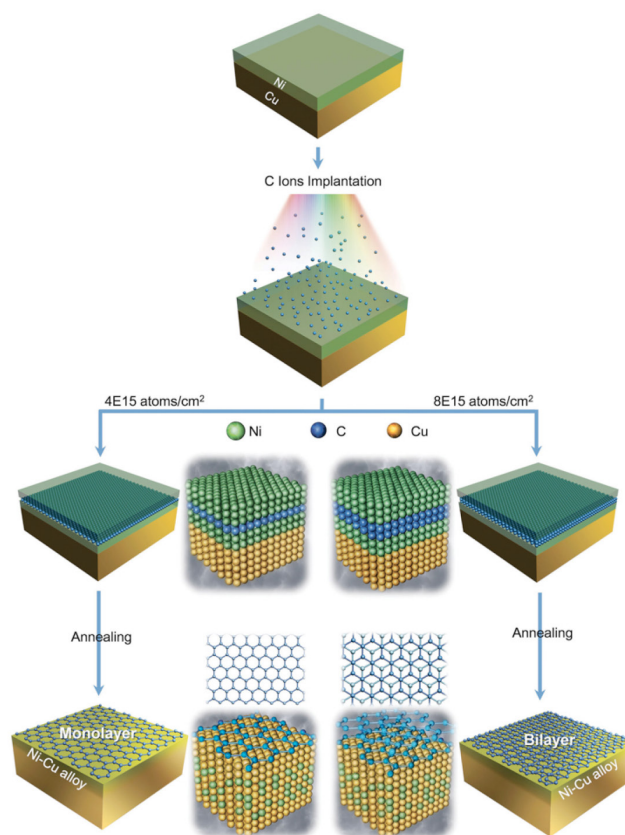
Authors are Yongqiang Wang (MST-8) and researchers from the Chinese Academy of Sciences, Lanzhou University, City

University of Hong Kong, Shanghai University, East China Normal University, and University at Buffalo - State University of New York.

The Center of Integrated Nanotechnologies, a DOE nanoscience user program jointly operated by Los Alamos and Sandia national laboratories, provided partial support. The Ion Beam Materials Laboratory is a multi-user research facility with multiple sponsors [DOE Basic Energy Sciences, DOE Nuclear Energy, Laboratory Directed Research and Development program, and the University of California Fees Research program].

The work supports the Laboratory's Energy Security mission area and Materials for the Future science pillar via advancement of the science to develop materials with properties optimized for specific functions and applications, such as nanoelectronics.

Technical contact: Yongqiang Wang



Schematic of the synthesis process to produce single-layer and double-layer graphene by ion implantation. Nickel (Ni) is depicted as green spheres, carbon (C) as blue, and copper (Cu) as yellow. Carbon ions with the pre-designed fluence were implanted into the top nickel layer of the Ni/Cu bilayer substrate followed by annealing. The thermal process initiates interdiffusion of Cu atoms and Ni atoms to form the Cu-like alloy. Carbon atoms are expelled from the Cu-like alloy toward the surface, and graphene with the expected layer number is formed on the surface.

HeadsUP!

Improving our work control systems

Call for micro-experiment solutions

Todd Conklin worked at Los Alamos National Laboratory for 26 years, leaving in 2012 to work as a safety consultant to help organizations better understand and improve their human performance. After the arc flash event here this summer, he returned to the Laboratory as a consultant. He reviewed the event and others and presented a talk to senior managers. He told the managers that the Laboratory needed to change its definition of success. There are two key quotes from his slides as related to work control:

- “We have conflicting missions: my success is based upon world-class science. Their success is based upon ZERO risk.”
- The second was a challenge to managers: “You have a duty to produce a different outcome: perfection cannot be the expectation; you must design your systems with the capacity to recover. This is a deliberate management strategy.”

Conklin recommended that we look at our systems and then try what he called micro-experiment solutions. In other words, we develop and try new ideas before we build huge systems.

To deliver world-class science, ADEPS is proposing to look at R&D skill-based activities, work that can be done without written instructions. The goal of the micro-experiment would be to identify in each group one skill-based work activity and to then convert the integrated work document for this class of activities to a one-pager.

Celebrating service

Congratulations to the following MST Division employees celebrating service anniversaries recently:

Esther Palluck, MST-8.....	30 years
Carl Trujillo, MST-8.....	30 years
Kendall Hollis, MST-6.....	20 years
James Valdez, MST-8.....	20 years
Franklin Fierro, MST-7.....	15 years
Markus Hehlen, MST-7.....	15 years
Joel Montalvo, MST-6.....	15 years
Sven Vogel, MST-8.....	15 years
Daniel Martinez, MST-8.....	10 years
Alice Smith, MST-16.....	10 years
John Carpenter, MST-6.....	5 years
Magdalena Serrano de Caro, MST-8.....	5 years

A call for volunteers was made and the first activity of the group, the ADEPS team, was a video conference with Lawrence Livermore National Laboratory staff on their new work control initiative. After the conference, the team compiled a list of positive and negative attributes of the system relative to the needs at Los Alamos. The concept of a skilled worker was well received to reduce the need for work documents and to address the idea of “skill of craft” for worker qualifications.

Another well-received idea, although it goes against the idea of huge systems, was that Livermore has an online system tracking all requirements: work control, training requirements, worker qualification, RLM approvals, etc.

Since the video teleconference, Los Alamos has initiated an institutional effort to look at the integrated work management system. Mary Hockaday is leading that effort. In a note to the volunteer group, she wrote, “If we are going to live up to our dream and accomplish our greatest imaginable challenge, we need to change the systems that are limiting our ability to perform efficiently.”

During the month of October, concurrent with the institutional effort, Hockaday has asked the team to brainstorm the biggest payoff activity we can do with our micro-experiment. If you have ideas or would like to join the team, please e-mail Howard Nekimken at hnek@lanl.gov.

MSTeNEWS

Materials Science and Technology

Published by the Experimental Physical Sciences Directorate

To submit news items or for more information, contact Karen Kippen, ADEPS Communications, at 505-606-1822, or kkippen@lanl.gov.

For past issues, see www.lanl.gov/org/padste/adeps/mst-e-news.php.



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LA-UR-15-28303

Approved for public release; distribution is unlimited.

Title: MST e-News October 2015

Author(s): Kippen, Karen Elizabeth

Intended for: Newsletter
Web

Issued: 2015-10-23

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